Optimization-Based Conservative Remap

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Background

Remap (Constrained Interpolation)

Given: Discrete representation u_A^h of u on mesh A.

Find: Accurate representation u_B^h of u on mesh B, subject to physical constraints:

- conservation of e.g. mass
- preservation of monotonicity
- optimal (arbitrary-order) accuracy
- physically meaningful ranges for variables: density ≥ 0, concentration $\in [0,1]$
- compatibility (*Schär and Smolarkiewicz*)

- Uses: transport, mesh rezone/repair, mesh tying, etc.
- Existing Lagrangian, Eulerian, ALE and particle-in-cell methods for CFD require **robust remap algorithms**.

Challenge: **Simultaneous** enforcement of constraints!

We have developed a new mathematical framework for the solution of remap problems, based on ideas from constrained optimization.

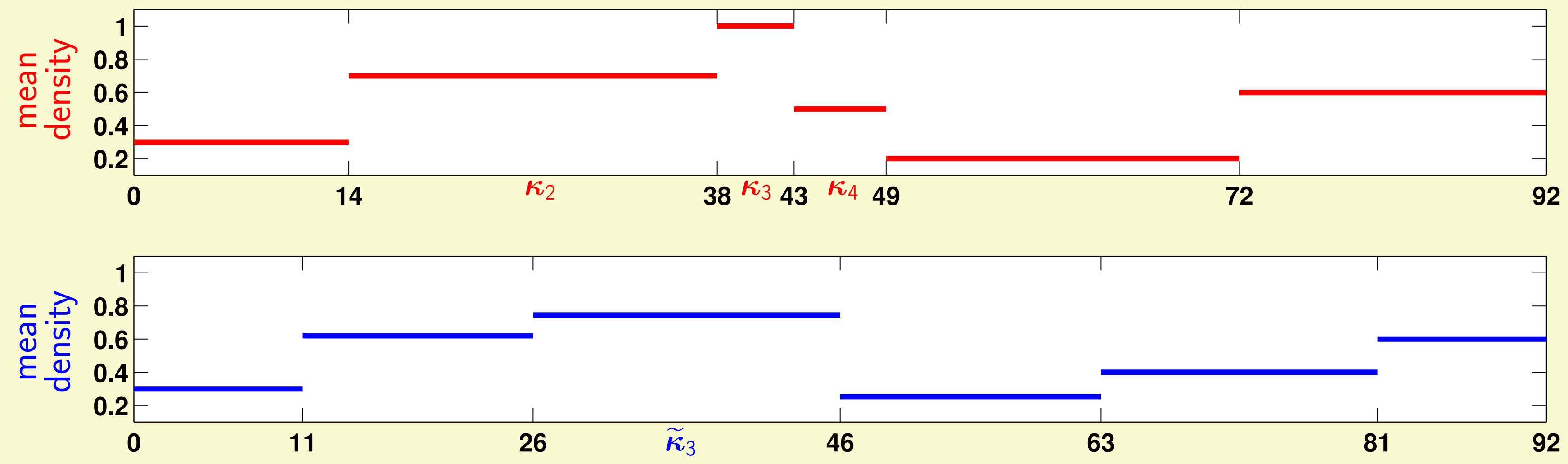
Goals:

- balancing of constraints: mass conservation, accuracy, monotonicity, bounds on variables, ...
- generality with respect to discretization: applicable to FE, FV and FD schemes as well as particle methods; suitable for arbitrary polyhedral grids!

Liska, Shashkov, et al., in "Optimization-Based Synchronized Flux-Corrected Remap" (J. C. Phys. 2010) pursue a **local** optimization approach.

We show that a **global** optimization strategy can have significant advantages!

Problem Setup for a Continuous Rezone Strategy



Notation:

- κ_i – cell in **old** grid, $\tilde{\kappa}_i$ – cell in **new** grid, K is # cells
- $E(\tilde{\kappa}_i)$ – neighborhood of $\tilde{\kappa}_i$ in old grid
- $\mathcal{I}(E(\tilde{\kappa}_i))$ – indices of neighbors of $\tilde{\kappa}_i$ in old grid

- mean values of density on old mesh: $\rho_i = \int_{\kappa_i} \rho(\mathbf{x})dV / V(\kappa_i)$
- masses: $m_i = \int_{\kappa_i} \rho(\mathbf{x})dV$ or $m_i = \rho_i V(\kappa_i)$
- total mass $M = \sum_{i=1}^K m_i$
- $\rho_i^{\min} \leq \rho_i \leq \rho_i^{\max} \quad \Leftrightarrow \quad \rho_i^{\min} V(\kappa_i) \leq m_i \leq \rho_i^{\max} V(\kappa_i)$

Remap of Mass-Density: Definition

Given mean density values ρ_i on the old grid cells κ_i, find accurate approximations $\widetilde{m}_i$ for the masses of the new grid cells $\tilde{\kappa}_i$:

$$\widetilde{m}_i \approx \widetilde{m}_i^{ex} = \int_{\tilde{\kappa}_i} \rho(\mathbf{x})dV\,; \quad i = 1,\ldots,K,$$

subject to the following constraints:

- Mass conservation: $\sum_{i=1}^K \widetilde{m}_i = \sum_{i=1}^K m_i = M$.
- 'Accuracy': For a globally linear density $\rho(\mathbf{x})$, the remapped masses are exact in the following sense: $\widetilde{m}_i = \widetilde{m}_i^{ex} = \int_{\tilde{\kappa}_i} \rho(\mathbf{x})dV\,; \quad i = 1,\ldots,K$.
- Bounds preservation (implies e.g. monotonicity): On every new cell $\tilde{\kappa}_i$: $\rho_i^{\min} \leq \tilde{\rho}_i \leq \rho_i^{\max}$ i.e. $\rho_i^{\min} V(\tilde{\kappa}_i) = \widetilde{m}_i^{\min} \leq \widetilde{m}_i \leq \widetilde{m}_i^{\max} = \rho_i^{\max} V(\tilde{\kappa}_i)$.

Remap of Mass-Density: Optimization Formulation

- Express new masses via the flux exchanges between old and new cells:

$$\widetilde{m}_i^{ex} = m_i + \sum_{j \in \mathcal{I}(E(\tilde{\kappa}_i))} F_{i,j}^{ex}\,, \text{ where } F_{i,j}^{ex} = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho(\mathbf{x})dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho(\mathbf{x})dV\,.$$

- Assume that for every *old* cell κ_i there is a density reconstruction ρ_i^h that is exact for linear functions. Define **target fluxes** according to

$$F_{i,j}^T = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho_j^h(\mathbf{x})dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho_i^h(\mathbf{x})dV\,.$$

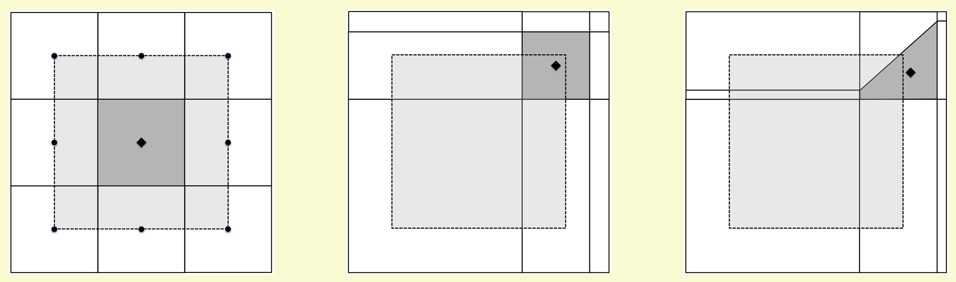
Optimization-Based Remap (OBR)

$$\underset{F_{i,j}^h}{\text{minimize}} \sum_{i=1}^K \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i<j}} (F_{i,j}^h - F_{i,j}^T)^2 \quad \text{subject to}$$

$$\widetilde{m}_i^{\min} \leq m_i + \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i<j}} F_{i,j}^h - \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i>j}} F_{j,i}^h \leq \widetilde{m}_i^{\max} \quad i = 1,\ldots,K.$$

Properties and Results

- Theorem (Linearity Preservation). A sufficient condition on mesh motion is that the centroid of any new cell remain inside the **convex hull** of the centroids of its old neighbors.

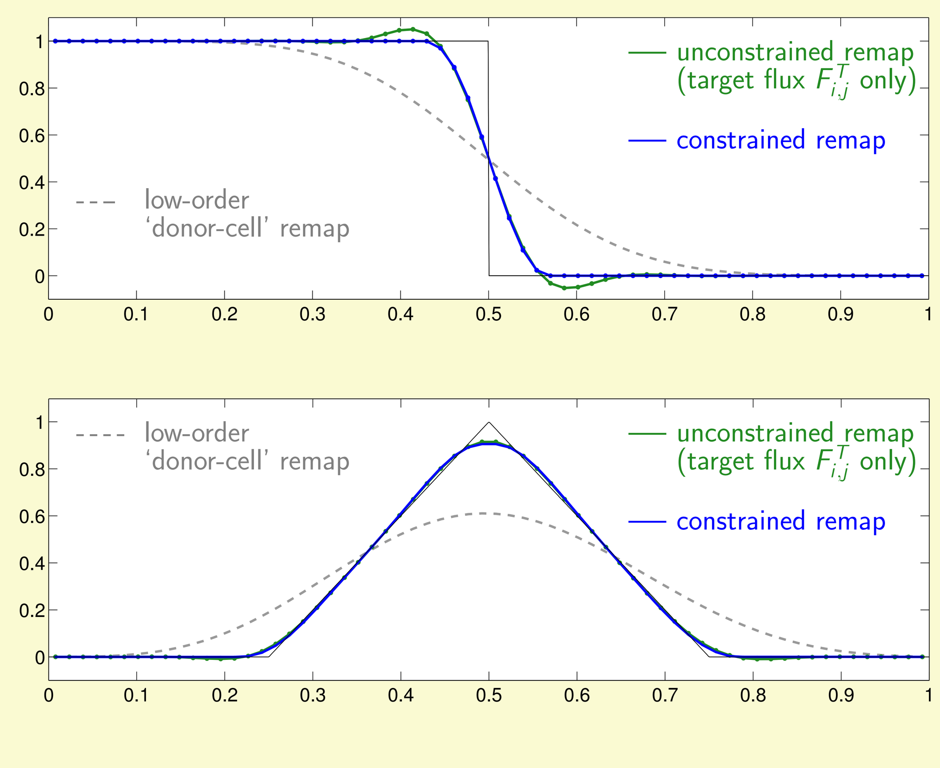


(a) original (b) admissible (c) inadmissible

- Bound preservation (monotonicity) is enforced explicitly.
- Optimally accurate with respect to a set distance measure.
- Permits additional physical bounds (just add constraints!).
- Extendible to compatible remap of systems (in progress).
- Separation of accuracy and monotonicity considerations!
- Clean formulation: **No limiters!**

'Shock' and 'Peak'

(Smooth mesh motion, $K = 64$, 320 remap steps)



Connection with the State of the Art. Example: Flux-Corrected Remap (FCR).

Theorem (FCR $\Rightarrow$ OBR). Flux-corrected remap (FCR) can be formulated as a (global) constrained optimization problem.
(1) The objective function of this optimization problem is equivalent to the objective function used in the OBR formulation.
(2) The feasible set of this optimization problem is **always a subset** of the feasible set of the OBR formulation.

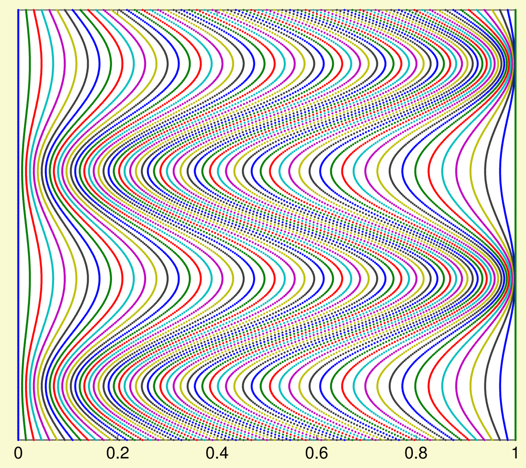
$$\text{OBR}\left\{\begin{array}{l} \underset{a_{i,j}}{\min} \sum_{i=1}^K \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i<j}} (1-a_{i,j})^2 (dF_{i,j})^2 \quad \text{subject to} \\ \widetilde{Q}_i^{\min} \leq \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i<j}} a_{i,j} dF_{i,j} - \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i>j}} a_{j,i} dF_{j,i} \leq \widetilde{Q}_i^{\max} \quad i = 1,\ldots,K \end{array}\right.$$

Admits a larger feasible set!

$$\text{FCR}\left\{\begin{array}{l} \underset{a_{i,j}}{\min} \sum_{i=1}^K \sum_{\substack{j \in \mathcal{I}(E(\tilde{\kappa}_i)) \\ i<j}} (1-a_{i,j})^2 (dF_{i,j})^2 \quad \text{subject to} \\ (a) \begin{cases} D_i^- dF_{i,j} \leq a_{i,j} dF_{i,j} \leq 0 & \text{for } i<j,\, dF_{i,j} \leq 0 \\ D_i^- dF_{j,i} \geq a_{j,i} dF_{j,i} \geq 0 & \text{for } i>j,\, dF_{j,i} \geq 0 \end{cases} \quad i = 1,\ldots,K \\ (b) \begin{cases} 0 \leq a_{i,j} dF_{i,j} \leq D_i^+ dF_{i,j} & \text{for } i<j,\, dF_{i,j} \geq 0 \\ 0 \geq a_{j,i} dF_{j,i} \geq D_i^+ dF_{j,i} & \text{for } i>j,\, dF_{j,i} \leq 0 \end{cases} \quad j \in \mathcal{I}(E(\tilde{\kappa}_i)) \end{array}\right.$$

Comparison with Flux-Corrected Remap, Part I

Smooth mesh motion

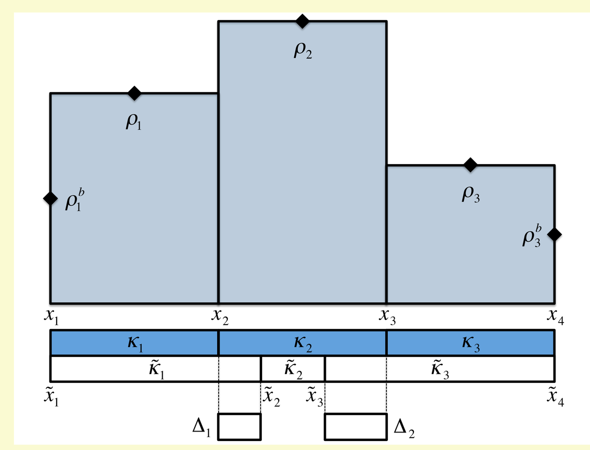


#cells	#remaps	'Sine' err	'Shock' err	'Peak' err	'Sine' rt	'Shock' rt	'Peak' rt
Optimization-Based Remap (OBR): L_1 error and convergence rate							
64	320	9.17e-4	2.47e-2	7.94e-3	—	—	—
256	1280	3.03e-5	8.97e-3	1.01e-3	2.47	0.73	1.49
1024	5120	9.30e-7	3.20e-3	1.27e-4	2.49	0.74	1.49
4096	20480	3.46e-8	1.15e-3	1.61e-5	2.46	0.74	1.49
Flux-Corrected Remap (FCR): L_1 error and convergence rate							
64	320	1.09e-3	2.47e-2	7.94e-3	—	—	—
256	1280	4.58e-5	8.87e-3	1.02e-3	2.29	0.74	1.49
1024	5120	2.17e-6	3.18e-3	1.31e-4	2.24	0.74	1.48
4096	20480	1.24e-7	1.15e-3	1.71e-5	2.19	0.74	1.48

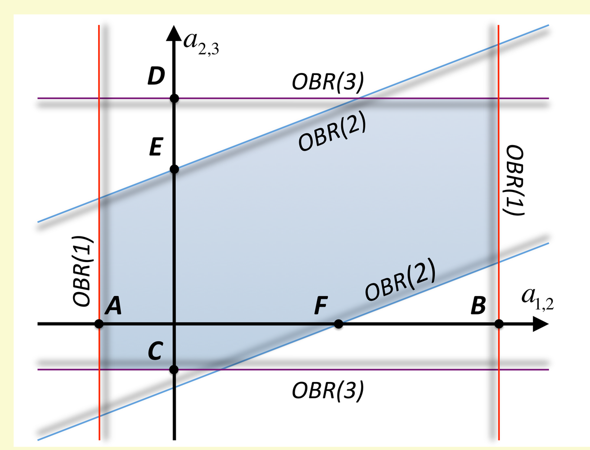
Virtually no difference in 'Shock' and 'Peak'; OBR exhibits a slightly better convergence rate for 'Sine'.

Comparison with Flux-Corrected Remap, Part II

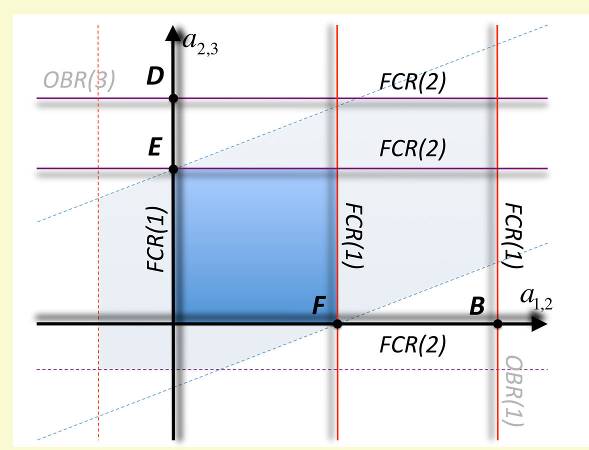
Compressive Mesh Motion

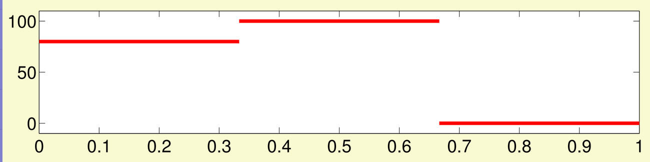


OBR Feasible Set (Cartoon)

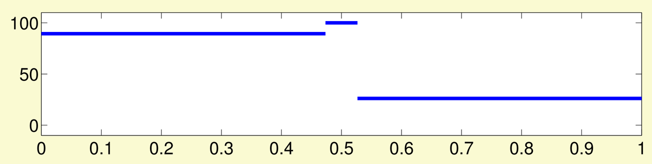


FCR Feasible Set (Cartoon)

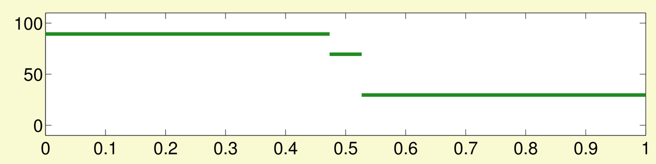




Original



After a single OBR step

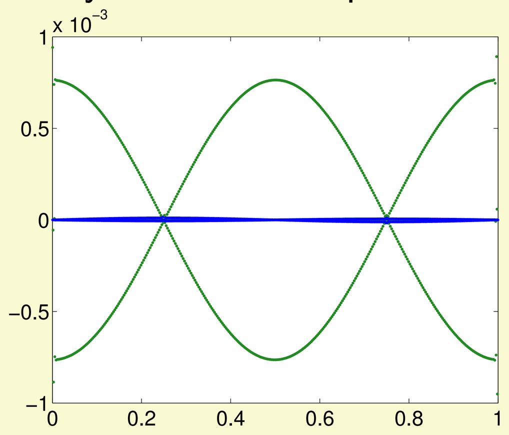


After a single FCR step

OBR preserves the original shape; FCR does not.

Error in 'Sine', $K = 1024$

Cyclic Mesh Compression



#cells	#remaps	L_2 err	L_1 err	L_∞ err	L_2 rate	L_1 rate	L_∞ rate
Optimization-Based Remap (OBR): L_2, L_1, L_∞ error and convergence rate							
64	320	1.52e-3	1.23e-3	3.87e-3	—	—	—
256	1280	8.96e-5	7.50e-5	2.44e-4	2.04	2.02	1.99
1024	5120	5.54e-6	4.68e-6	1.54e-5	2.03	2.01	1.99
4096	20480	3.45e-7	2.93e-7	1.39e-6	2.02	2.01	1.92
Flux-Corrected Remap (FCR): L_2, L_1, L_∞ error and convergence rate							
64	320	7.71e-3	5.96e-3	1.57e-2	—	—	—
256	1280	1.78e-3	1.31e-3	3.81e-3	1.06	1.09	1.02
1024	5120	4.42e-4	3.25e-4	9.51e-4	1.03	1.05	1.01
4096	20480	1.10e-4	8.10e-5	2.38e-4	1.02	1.03	1.01

OBR exhibits best expected rate, 2[nd] order; FCR is only 1[st] order accurate!

Computational Feasibility (1D Results)

- The optimization problem can be reformulated as a box-constrained QP with a single equality constraint.
- Solved using a penalty formulation and a finely tuned Newton-type method based on Coleman/Hulbert (1993).
- Redundant (fixed) variables are recognized and eliminated automatically → **physics-aware computation**.
- **Fast linear algebra enables $\mathcal{O}(K)$ complexity.**

	# cells	# remaps	FCR(sec)	OBR(sec)	ratio
'Sine' worst case!	262,144	10	6.35	43.11	6.8
	524,288	10	12.60	85.56	6.8
	1,048,576	10	25.33	165.67	6.5

	# cells	# remaps	FCR(sec)	OBR(sec)	ratio
'Shock'	262,144	10	6.12	5.28	0.86
	524,288	10	12.11	10.07	0.83
	1,048,576	10	23.76	19.77	0.83

References

P. Bochev, D. Ridzal, G. Scovazzi, M. Shashkov, *Formulation, analysis and computation of an optimization-based conservative, monotone and bounds-preserving remap of scalar fields*, SAND Report, 2010.

R. Liska, M. Shashkov, P. Váchal, B. Wendroff, *Optimization-based synchronized flux-corrected conservative remapping of mass and momentum for ALE methods*, 229(5):1467-1497, J. Comp. Phys., 2010.

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